

Special Issue

Configurational Entropy

Message from the Guest Editor

Changes in the configurational part of entropy contribute significantly to the free energy of conformational change and binding in biomolecular systems. In particular, the change in configurational entropy is an important determinant of the energetics of the binding affinity in receptor-ligand systems. However, calculating the configurational entropy of complex non-harmonic systems is a highly challenging problem in need of innovative approaches to a practicable solution. Recently, information-theoretic methods and nonparametric statistical methods have been brought to bear on the problem of estimating configurational entropy from molecular simulations. This special issue of Entropy will provide a forum for contributions on both theoretical and computational aspects of the entropic characteristics of complex systems.

Guest Editor

Dr. Vladimir Hnizdo

National Institute for Occupational Safety and Health, Morgantown, WV
26505, USA

Deadline for manuscript submissions

closed (30 April 2010)



Entropy

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CiteScore 4.9
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Entropy
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
entropy@mdpi.com

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About the Journal

Message from the Editor-in-Chief

The concept of entropy is traditionally a quantity in physics that has to do with temperature. However, it is now clear that entropy is deeply related to information theory and the process of inference. As such, entropic techniques have found broad application in the sciences.

Entropy is an online open access journal providing an advanced forum for the development and/or application of entropic and information-theoretic studies in a wide variety of applications. *Entropy* is inviting innovative and insightful contributions. Please consider *Entropy* as an exceptional home for your manuscript.

Editor-in-Chief

Prof. Dr. Kevin H. Knuth

Department of Physics, University at Albany, 1400 Washington Avenue,
Albany, NY 12222, USA

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